

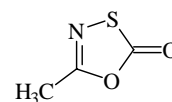
1122
ED, MW

C₃H₃NO₂S

5-Methyl-1,3,4-oxathiazol-2-one

C_s

r_a	Å ^{a)}	θ_α	deg ^{a)}
O(1)–C(2)	1.391(6)	C(5)–O(1)–C(2)	111.8(3)
O(1)–C(5)	1.367(9)	O(1)–C(2)=O(6)	123.6(4)
S(3)–C(2)	1.768(2)	C(2)–S(3)–N(4)	93.5(2)
S(3)–N(4)	1.685(2)	O(1)–C(5)–C(7)	115.3(4)
N(4)=C(5)	1.289(4)	C–C–H	109.6(5)
C(2)=O(6)	1.198(2)	O(1)–C(2)–S(3) ^{b)}	106.4(3)
C(5)–C(7)	1.487(3)	O(1)–C(5)=N(4) ^{b)}	119.3(2)
C–H	1.102(30)	C(5)=N(4)–S(3) ^{b)}	109.2(3)
		τ ^{c)}	0 ^{d)}



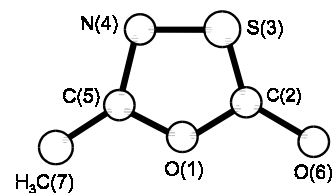
The nozzle temperature was 62 °C.

^{a)} Estimated standard errors.

^{b)} Dependent parameter.

^{c)} Dihedral angle N(4)=C(5)–C(7)–H.

^{d)} Fixed.



Bak, B., Nielsen, O., Svanholt, H., Almenningen, A., Bastiansen, O., Braathen, G.,
Fernholt, L., Gundersen, G., Nielsen, C.J., Cyvin, B.N., Cyvin, S.J.: Acta Chem. Scand.
Ser. A **36** (1982) 283.